

## Ecotox Report for Case # P-19-0138

### General

<b>CBI:</b> [REDACTED]	<b>Report Status:</b> Complete
<b>Status Date:</b> 04/29/2020	<b>CRSS Date:</b> 08/05/2019
<b>SAT Date:</b> 08/12/2019	<b>SAT Chair:</b> Jeffrey Gallagher
<b>Consolidated</b> N	<b>Consolidated Set:</b>
<b>PMN:</b>	
<b>Ecotox Related</b>	[REDACTED]
<b>Cases:</b>	
<b>Health Related</b>	
<b>Cases:</b>	
<b>Submitter:</b>	[REDACTED]
<b>CAS Number:</b>	[REDACTED]
<b>Chemical Name:</b>	[REDACTED]
<b>Use:</b> Intended use	intermediate
	[REDACTED]
	Synthetic scheme
	Analogues (same use):
	[REDACTED]
	Patents (same use):
	[REDACTED]
<b>Trade Name:</b>	[REDACTED]
<b>PV max(kg/yr):</b>	[REDACTED]
	<b>Ecotox Assessor:</b> Kim, Anne

### Fate Summary Statement

#### Fate Summary P 19 0138

**Statement:** FATE: Estimations for hydrolysis product acid, MW = [REDACTED] [REDACTED]

S Reacts

Hydrolysis Half-life  $\leq$  min

VP [REDACTED] torr at [REDACTED] °C (NOMO5)

BP = [REDACTED] °C (M)

POTW removal (%) PMN 90 99 via hydrolysis; then Hyd Pdt [REDACTED]

[REDACTED] 0;

Hyd Pdt HF 60 via sorption

Time for complete ultimate aerobic biodeg = Hyd Pdt [REDACTED] > mo;

Hyd Pdt HF mo

Sorption to soils/sediments = Hyd Pdt [REDACTED] low; Hyd Pdt HF moderate

PBT Potential: PMN P1B1; Hyd Pdt [REDACTED] P3BU; Hyd Pdt HF P3B1

FATE: Migration to ground water = PMN negl; Hyd Pdt [REDACTED] rapid;  
Hyd Pdt HF moderate

Analogue found (include identifier and database)

Relevant Structure(s)

Landfill [REDACTED] product and [REDACTED]

Air / Incineration Parent

Parent % incineration 99.9% (hazardous waste incinerator)

Environmental Fate Determination

PMN #: P-19-0138

Summary: EPA estimated that the new chemical substance could have limited persistence and a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. The hydrolysis product [REDACTED] is estimated to be very persistent in the environment and its bioaccumulation potential is unknown; therefore, it is not known whether repeated exposures to it will cause food chain effects via accumulation in exposed organisms. Although EPA estimated that the hydrolysis product [REDACTED] could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of the new chemical substance using data for analogues ([REDACTED]); of the hydrolysis product [REDACTED] using data for analogue(s) [REDACTED], and data submitted for the hydrolysis product; and of the hydrolysis product ([REDACTED] using data available for [REDACTED] and fluoride ions. In wastewater treatment, the new chemical substance is expected to be removed with an efficiency of 90% to 99% due to rapid hydrolysis, the hydrolysis product [REDACTED] is expected to be removed with an efficiency of 0% due to low biodegradability, low sorption, and low stripping, and the hydrolysis product ([REDACTED] is expected to be removed with an efficiency of 60% due to sorption. Removal of the hydrolysis products ([REDACTED] by biodegradation is negligible. Sorption of the hydrolysis product [REDACTED] to sludge, soil, and sediment is expected



to be low and sorption of the hydrolysis product ( ) to sludge, soil, and sediment is expected to be moderate. Migration of the new chemical substance to groundwater is expected to be negligible due to rapid hydrolysis, migration of the hydrolysis product ( ) to groundwater is expected to be rapid due to low sorption to soil and sediment, and migration of the hydrolysis product ( ) to groundwater is expected to be moderate due to moderate sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the new chemical substance and the hydrolysis product ( ) are expected to undergo negligible volatilization to air. Due to low reported vapor pressure, the hydrolysis product ( ) is expected to undergo negligible volatilization to air. Overall, these estimates indicate that the new chemical substance has low potential to volatilize to air or migrate to groundwater; that the hydrolysis product ( ) has low potential to volatilize to air and has high potential to migrate to groundwater; and that the hydrolysis product ( ) has low potential to volatilize to air and has moderate potential to migrate to groundwater.

**Persistence :** Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human health or the environment. EPA estimated degradation half-lives of the new chemical substance using data for analogues ( ), of the hydrolysis product ( ) using data for analogue(s) ( ), and of the hydrolysis product ( ) using data available for ( ). EPA estimated that the new chemical substance's hydrolysis half-life is seconds; that the hydrolysis products' ( ) aerobic and anaerobic biodegradation half-lives are > 6 months. These estimates indicate that the new chemical substance may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediments) due to hydrolysis. Further, these estimates indicate that the hydrolysis products ( ) and ( ) may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

**Bioaccumulation :** Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via food chains. EPA estimated the potential for the new chemical substance to bioaccumulate using data for analogues ( ) and of the hydrolysis product ( ) to bioaccumulate using data for fluoride ions. EPA estimated that the new chemical substance has low bioaccumulation potential based on rapid hydrolysis, the hydrolysis product ( ) has unknown bioaccumulation potential based on bioconcentration or

bioaccumulation data reported for highly fluorinated aliphatic chemicals, and the hydrolysis product ( ) has low bioaccumulation potential based on fluoride, which is a nutrient. EPA estimated that the new chemical substance could have limited persistence and a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. The hydrolysis product ( ) is estimated to be very persistent in the environment and its bioaccumulation potential is unknown; therefore, it is not known whether repeated exposures to it will cause food chain effects via accumulation in exposed organisms. Although EPA estimated that the hydrolysis product ( ) could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

## Physical Chemical Information

<b>Molecular Weight:</b>	
<b>Wt% &lt; 500:</b>	<b>Wt% &lt; 1000:</b>
<b>Physical State - Neat:</b>	
<b>Melting Point: MP (EPI):</b>	<b>Melting Point (est):</b>
<b>Vapor Pressure: VP (EPI):</b>	<b>Vapor Pressure (est):</b>
<b>Water Solubility: Water Solubility (EPI):</b>	<b>Water Solubility (est):</b>
<b>Henry's Law::</b>	
<b>Log Koc: NaN</b>	<b>Log Koc (EPI):</b>
<b>Log Kow:</b>	<b>Log Kow (EPI):</b>
<b>Log Kow</b>	
<b>Comment:</b>	

## SAT Concern Level

<b>Ecotox Rating (1):</b>
<b>Ecotox Rating Comment (1):</b>
<b>Ecotox Rating (2):</b>
<b>Ecotox Rating</b>



**Comment (2):**  
**Ecotox Route of Exposure:** All releases to water

## Ecotox Comments

**Exposure Based Review (Eco):**  
**Ecotox Comments:**  
**Exposure Based Testing:**

## PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1	1		PMN
3	U		Hyd Pdt [REDACTED]
3	1		Hyd Pdt HF

## Eco-Toxicity Comment:

## Fate Ratings

Removal in 90-99;0;60 PMN;Hyd Pdt [REDACTED] Hyd Pdt HF							
<b>WWT/POTW (Overall):</b>							
<b>Condition</b>	<b>Rating Values</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>Comment</b>	
<b>Fish BCF:</b>							
<b>Log Fish BCF:</b>							
<b>WWT/POTW Sorption:</b>	;1;2	Low	Moderate	Strong	V. Strong	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF	
<b>WWT/POTW Stripping:</b>	4;4;4	Extensive	Moderate	Low	Negligible	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF	
<b>Biodegradation Removal:</b>	;4;4	Unknown	High	Moderate	Negligible		

Removal in 90-99;0;60 PMN;Hyd Pdt [REDACTED] Hyd Pdt HF  
 WWT/POTW  
 (Overall):

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	;4;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	;4;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	[REDACTED]
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	;4;3	V. Strong	Strong	Moderate	Low	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF
Migration to Ground Water:	1;4;3	Negligible	Slow	Moderate	Rapid	PMN;Hyd Pdt [REDACTED] Hyd Pdt HF
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Removal in 90-99;0;60 PMN;Hyd Pdt [REDACTED] Hyd Pdt [REDACTED]  
 WWT/POTW

(Overall):

Condition	Rating	Rating Description				Comment
	Values	1	2	3	4	

**Bio Comments:** Fate Study Summaries are available.

The substance will hydrolyze (sec) to yield [REDACTED] and the acid hydrolysis product [REDACTED]

The fugacity spreadsheet and the EPI output file for the carboxylic acid hydrolysis product of the PMN material are attached.

**Fate Comments:**

## Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	> 96.9		Predictions are based on analogue test data ([REDACTED])
Daphnid	48-h	LC50	> 102		Predictions are based on analogue test data ([REDACTED])
Green Algae	96-h	EC50	> 106		Predictions are based on analogue test data ([REDACTED])
Fish	-	Chronic Value	1.53		Predictions are based on analogue test data ([REDACTED])
Daphnid	-	Chronic Value	5.82		Predictions are based on analogue test data ([REDACTED])
Green Algae	-	Chronic Value	> 106		Predictions are based on analogue test data ([REDACTED])

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Avian		Chronic Value	> 950		Predictions are based on analogue test data ( )
<b>Ecotox Value</b> Predictions are based on analogue test data ( ) MW Log <b>Comments:</b> Kow = (M, Hyd Pdt); liquid with an unknown MP (P); S = (M, PMN), (P, Hyd Pdt); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO <sub>3</sub> ; and TOC <2.0 mg/L.					

## Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic(ppb):	> 96.9	5	> 19,380	Fish LC50
Chronic Aquatic(ppb):	1530	10	153	Fish ChV

Factors	Values	Comments
SARs:		
SAR Class:		
TSCA NCC Category?	None	

## Recommended Testing:

**Ecotox Factors** Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data on analogous chemicals. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are > 96.9 mg/L, > 102 mg/L, and > 106 mg/L, respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are 1.53 mg/L, 5.82 mg/L, and > 106 mg/L, respectively. These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of > 19.38 mg/L (> 19,380 ppb) and 0.153 mg/L (153 ppb), respectively.



Environmental Risk: Risks to the environment were not identified due to no releases to water.

## Comments/Telephone Log

Artifact	Update/Upload Time
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